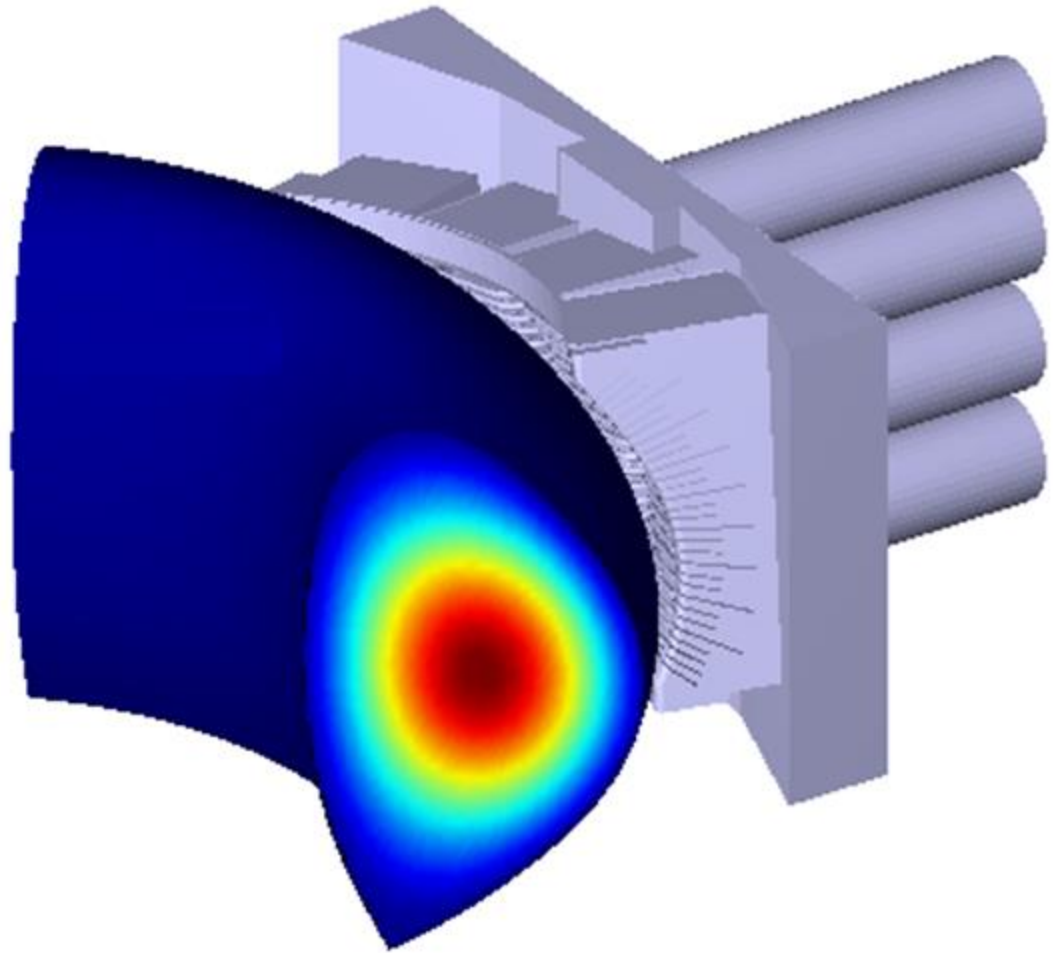


Coupling of VSim RF code with BOUT++ in RF SciDAC-4

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BOUT++ Workshop
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LLNL



(This is a preview of my APS poster)

Computing tensor ponderomotive force terms in Vorpal for use in BOUT++

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A literature survey across numerous references discussing ponderomotive force leads us to a single consolidated formulation, utilizing the fluid force equation and separation of time-scales. We present analytical case studies from various scenarios of the formulation where ponderomotive forces can occur. Of significance is that this work includes the presence of collisions with neutral gas (RF drag and absorption) in the far-SOL and partial ionization regions. The formulation includes a classical term with $\nabla|V_{RF}|^2$, thus permitting force in non-drift directions. Other terms include cyclotron motion and neutral gas collisions, and have gradients of plasma and neutral gas density, and thus can be significant in the steep density gradients. We implement diagnostic calculation of these ponderomotive forces in the Vorpal time-domain plasma model, and starting from the description of the BOUT equations in

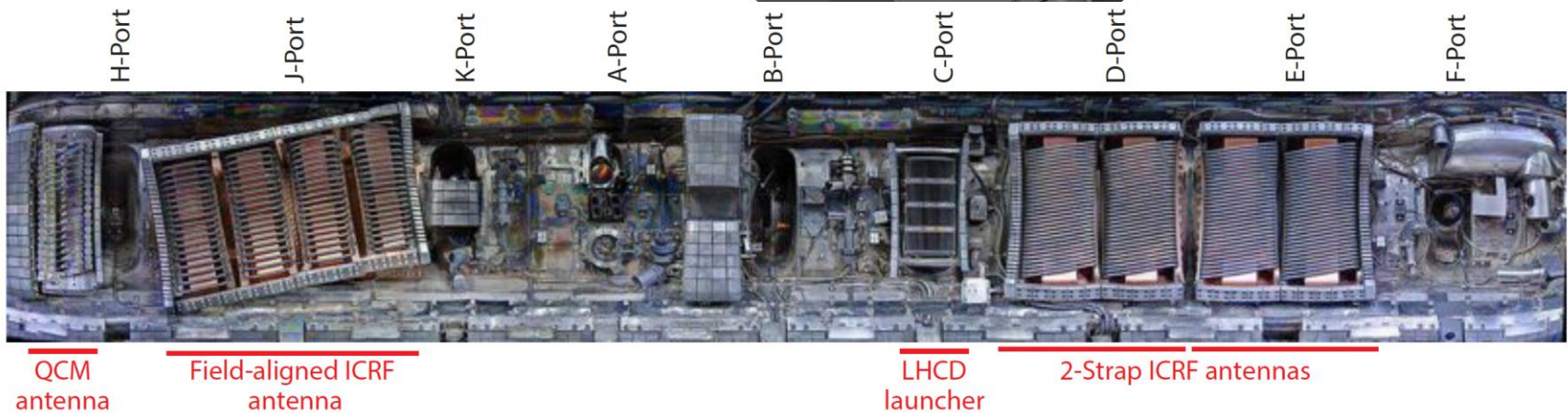
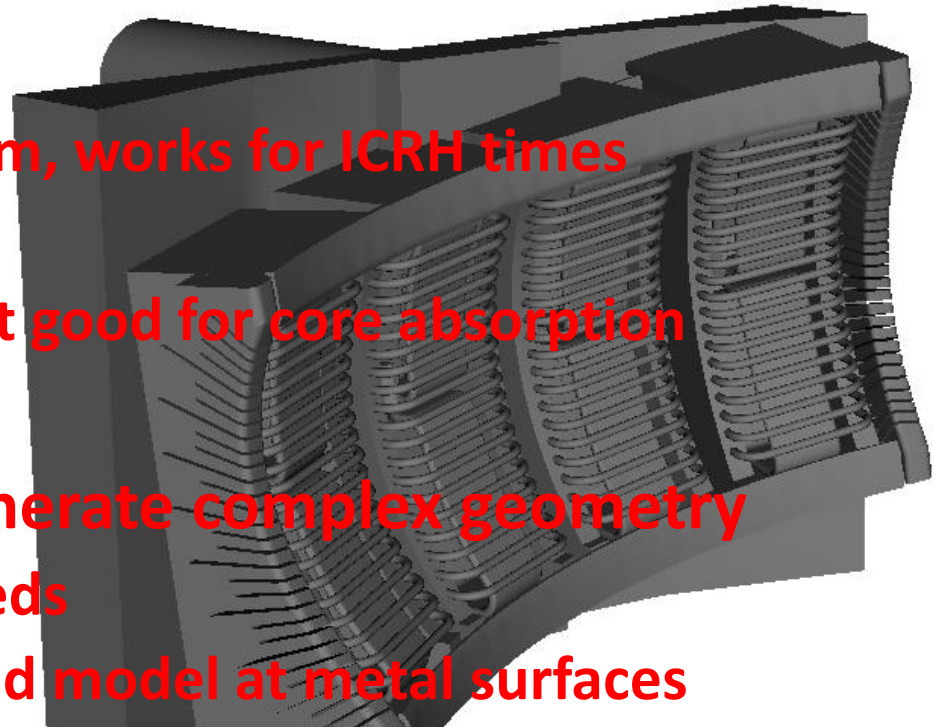
What is VSim?

- **3D-FDTD-EM-PIC**

- Cold plasma fluid algorithm, works for ICRH times
- No PIC particles for this!
- Good for edge plasma, not good for core absorption

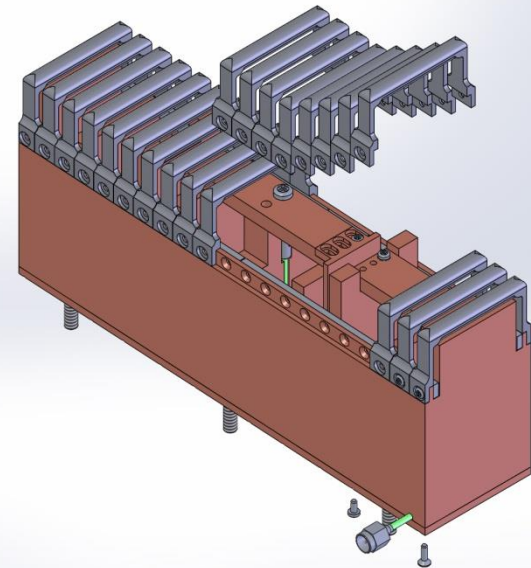
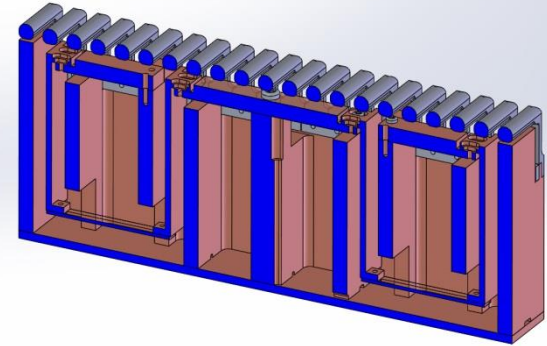
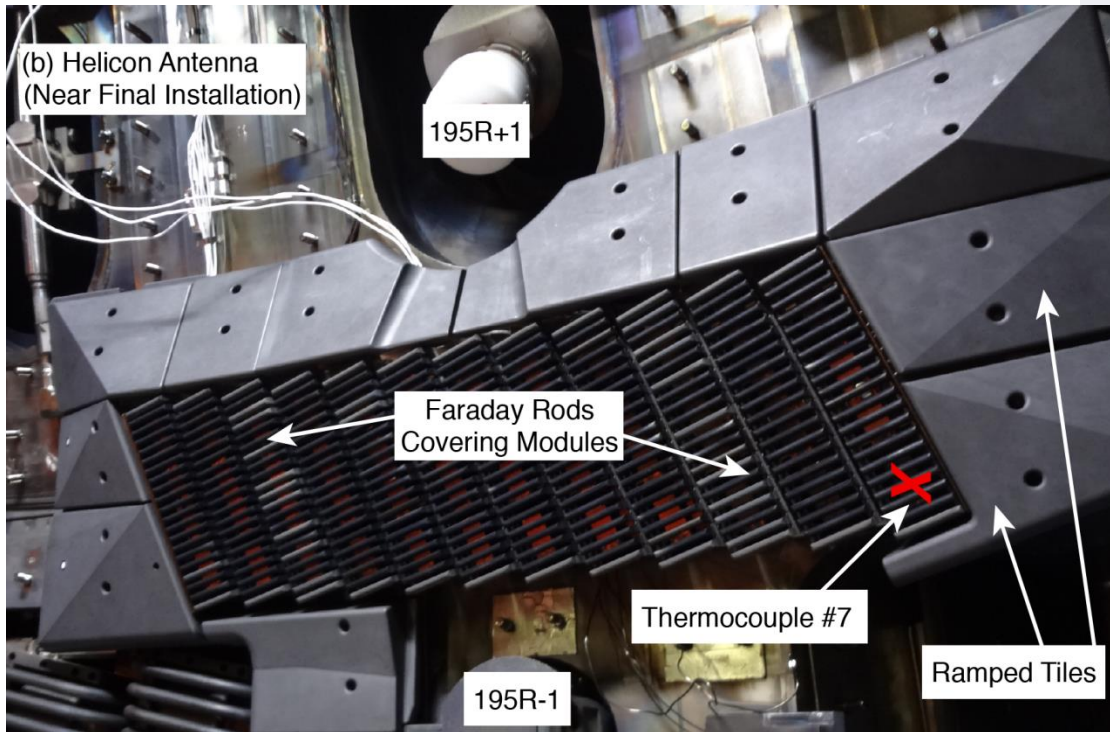
- **Import 3D CAD files or generate complex geometry**

- Include the waveguide feeds
- Includes RF sheath sub-grid model at metal surfaces



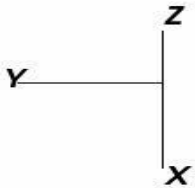
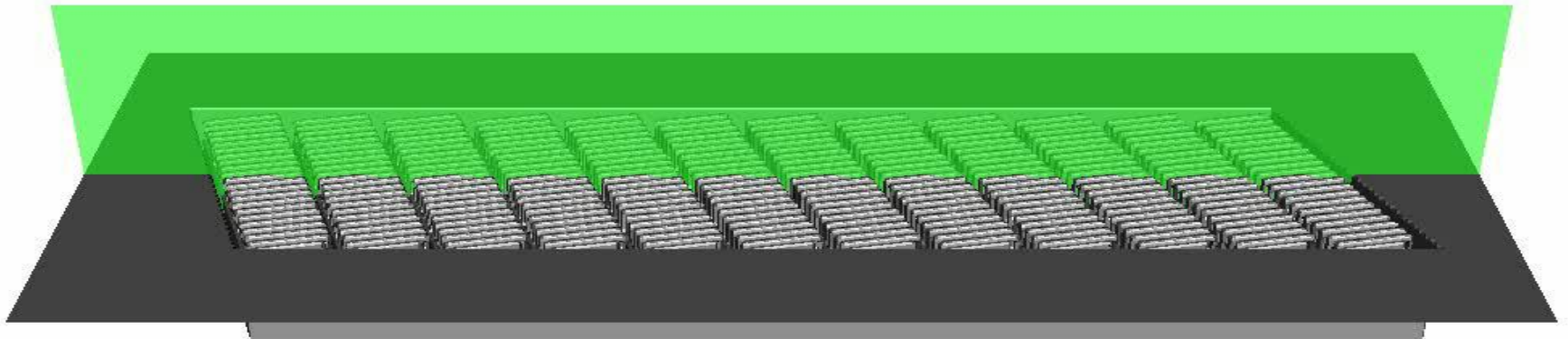
Example: CMod FA-ICRF antenna

Example: DIII-D Helicon (Low Power)



Helicon Antenna Operation

- Only the end module is powered, remaining modules couple inductively.



RF Plasma Algorithm in VSim

- VSim already does Maxwell's equations: \mathbf{E} , \mathbf{B}
- Need \mathbf{B}_0 field.
- Need fields for each species: ρ_{s0} , \mathbf{J}_{s1}
- Also have collision frequency, ν_s .
 - Artificial resonance broadening in core
 - Artificial wave absorber at simulation boundary
 - Realistic neutral gas at edge

BOUT++ (slow) \Leftrightarrow VSim (fast)

- **Slow₀ Time Scale (lo-pass filter)**

Extra Slow Force !

$$\begin{aligned}
 {}^{(m/q)}_s \left[\begin{array}{c} \partial_t \mathbf{J}_{s0} + \nabla \cdot [\mathbf{J}_{s0} \mathbf{J}_{s0} / \rho_{s0}] \\ \rho_{s0} \{ \partial_t + \mathbf{V}_{s0} \cdot \nabla \} \mathbf{V}_{s0} \end{array} \right] + \nabla \cdot [\mathbb{P}_{s0}] &= \left[\begin{array}{c} \rho_{s0} \mathbf{E}_0 + \mathbf{J}_{s0} \times \mathbf{B}_0 \\ \rho_{s0} (\mathbf{E}_0 + \mathbf{V}_{s0} \times \mathbf{B}_0) \end{array} \right] + \langle \mathbf{F}_s \rangle_{lo-pass} \\
 &+ \langle Collisions \rangle_{lo-pass} + \langle Sources \rangle_{lo-pass}
 \end{aligned}$$

- **Fast₁ Time Scale (hi-pass filter)**

$$\begin{aligned}
 {}^{(m/q)}_s \partial_t \mathbf{J}_{s1} + {}^{(m/q)}_s \nabla \cdot [\mathbf{V}_{s0} \mathbf{J}_{s1} + \mathbf{J}_{s1} \mathbf{V}_{s0} - \rho_{s1} \mathbf{V}_{s0} \mathbf{V}_{s0}] + \nabla \cdot \mathbb{P}_{s1} &= \\
 \rho_{s0} \mathbf{E}_1 + \rho_{s1} \mathbf{E}_0 + \mathbf{J}_{s0} \times \mathbf{B}_1 + \mathbf{J}_{s1} \times \mathbf{B}_0 + \langle \mathbf{F}_s \rangle_{hi-pass} & \\
 + \langle Collisions \rangle_{hi-pass} + \langle Sources \rangle_{hi-pass} &
 \end{aligned}$$

The (Extra) Ponderomotive Force

- It's just all the products of two fast-time scale quantities in fluid equation:

$$\mathbf{F}_s \equiv \rho_{s1} \mathbf{E}_1 + \mathbf{J}_{s1} \times \mathbf{B}_1 - \left(\frac{m}{q} \right)_s \nabla \cdot \left[\frac{\rho_{s0}^2 \mathbf{V}_{s1} \mathbf{V}_{s1}}{\rho_{s0} + \rho_{s1}} \right]$$

$$\mathbf{J}_{s1} = \rho_{s0} \mathbf{V}_{s1} + \rho_{s1} \mathbf{V}_{s0}$$

- Lee & Parks Form (single frequency):

$$\mathbf{F}_s = -\rho_{s0} \nabla (\psi_p / Ze) + \mathbf{B} \times (\nabla \times \mathbf{M})$$

$$\psi_p / Ze = - \frac{1}{4} \text{Imag} \{ \mathbf{u}^* \cdot \mathbf{E} \} / \omega$$

$$\mathbf{M} = \frac{1}{4} \rho_{s0} \text{Imag} \{ \mathbf{u}^* \times \mathbf{u} \} / \omega \quad -i\omega \mathbf{u} - \mathbf{u} \times \boldsymbol{\Omega}_s = \left(\frac{q}{m} \right)_s \mathbf{E}$$

The Ponderomotive Force (Again)

- VSim will indeed take the lo-pass filter of

$$\mathbf{F}_s \equiv \rho_{s1} \mathbf{E}_1 + \mathbf{J}_{s1} \times \mathbf{B}_1 - (m/q)_s \nabla \cdot \left[\frac{\rho_{s0}^2 \mathbf{V}_{s1} \mathbf{V}_{s1}}{\rho_{s0} + \rho_{s1}} \right]$$

- Qualitative Understanding from

(In time for APS!)

$$\mathbf{F}_s = -\rho_{s0} \nabla (\psi_p / Ze) + \mathbf{B} \times (\nabla \times \mathbf{M})$$

- First term is gradient of (mostly positive) “wave pressure”
- Second term is ... well ... extra.
- \mathbf{M} is non-zero for circularly polarized \mathbf{V}_{s1} .

Ponderomotive Force in BOUT++

Appendix A. Summary of BOUT equations

A.1. Electron parallel momentum

$$\begin{aligned} \frac{\partial V_{\parallel e}}{\partial t} + (\vec{V}_E + V_{\parallel e} \vec{b}_0) \cdot \nabla V_{\parallel e} = & -\frac{e}{m_e} E_{\parallel} - \frac{1}{N_i m_e} (T_e \partial_{\parallel} N_i + 1.71 N_i \partial_{\parallel} T_e) \\ & + 0.51 v_{ei} (V_{\parallel i} - V_{\parallel e}) - \frac{1}{N_i m_e} \frac{2}{3} B^{3/2} \partial_{\parallel} (B^{-3/2} (P_{\parallel e} - P_{\perp e})) + \boxed{\frac{S_{\parallel e}^m}{N_i m_e}} + \frac{S_e^p}{N_i} V_{\parallel e}. \end{aligned}$$

A.2. Vorticity

$$\begin{aligned} \frac{\partial \varpi}{\partial t} + (\vec{V}_E + V_{\parallel i} \vec{b}_0) \cdot \nabla \varpi = & (2\omega_{ci}) \vec{b}_0 \times \vec{k} \cdot \left(\nabla P + \frac{1}{6} \nabla (P_{\parallel i} - P_{\perp i}) \right) \\ & + N_i Z_i e \frac{4\pi V_A^2}{c^2} \nabla_{\parallel} j_{\parallel} + \mu_{ii} \nabla_{\perp}^2 \varpi - (B\omega_{ci}) \nabla \cdot \left(\frac{\vec{b}_0}{B} \times (S_e^m + S_i^m) \right) - \left(\frac{S_i^p}{N_i} \right) \varpi \\ & - (\omega_{ci} B) \nabla \left(\frac{S_i^p}{N_i \omega_{ci} B} \right) \cdot (N_i Z_i e \nabla \phi + \nabla P_i) - \frac{1}{2} [N_i q V_{pi} \cdot \nabla (\nabla_{\perp}^2 \phi) \\ & - M_i \omega_{ci} \vec{b} \times \nabla N_i \cdot \nabla \vec{V}_E^2] + \frac{1}{2} [\vec{V}_E \cdot \nabla (\nabla_{\perp}^2 P_i) - \nabla_{\perp}^2 (\vec{V}_E \cdot \nabla P_i)]. \end{aligned}$$

A.3. Density

$$\frac{\partial N_i}{\partial t} + (\vec{V}_E + V_{\parallel i} \vec{b}_0) \cdot \nabla N_i = \left(\frac{2c}{eB} \right) \vec{b}_0 \times \vec{k} \cdot (\nabla P_e - N_i e \nabla \phi) + \nabla_{\parallel} \left(\frac{j_{\parallel}}{e} \right) - N_i \nabla_{\parallel} V_{\parallel i} + S_e^p.$$

A.4. Ion temperature

$$\begin{aligned} \frac{\partial T_i}{\partial t} + (\vec{V}_E + V_{\parallel i} \vec{b}_0) \cdot \nabla T_i = & \frac{4}{3} \left(\frac{c T_i}{N_i e B} \right) \vec{b}_0 \times \vec{k} \cdot (\nabla P_e - N_i e \nabla \phi - \frac{5}{2} N_i \nabla T_i) \\ & + \frac{2}{3 N_i} \nabla_{\parallel} (\kappa_{\parallel i}^c \partial_{\parallel} T_i) + \boxed{\frac{2 S_i^E}{3 N_i}} - \frac{2 T_i}{3 N_i} \left(N_i \nabla_{\parallel} V_{\parallel i} - \frac{1}{e} \nabla_{\parallel} j_{\parallel} \right) \\ & + \frac{2 m_e}{m_i} v_{ei} (T_e - T_i) + \frac{2}{3} \left(\frac{20}{3} \mu_{ii} \right) \nabla_{\perp}^2 T_i - v_i T_i. \end{aligned}$$

A.5. Electron temperature

$$\begin{aligned} \frac{\partial T_e}{\partial t} + (\vec{V}_E + V_{\parallel e} \vec{b}_0) \cdot \nabla T_e = & \frac{4}{3} \left(\frac{c T_e}{N_i e B} \right) \vec{b}_0 \times \vec{k} \cdot (\nabla P_e - N_i e \nabla \phi + \frac{5}{2} N_i \nabla T_e) \\ & + \frac{2}{3 N_i} \nabla_{\parallel} (\kappa_{\parallel e}^c \partial_{\parallel} T_e) + \frac{2 \eta_{\parallel}}{2 N_i} j_{\parallel}^2 - \frac{2 T_e}{3} \nabla_{\parallel} V_{\parallel e} - \frac{2 m_e}{m_i} v_{ei} (T_e - T_i) \\ & + 0.71 \frac{2 T_e}{3 N_i e} \nabla_{\parallel} j_{\parallel} + \boxed{\frac{2 S_e^E}{3 N_i}} - v_i T_e. \end{aligned}$$

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Computer Physics Communications

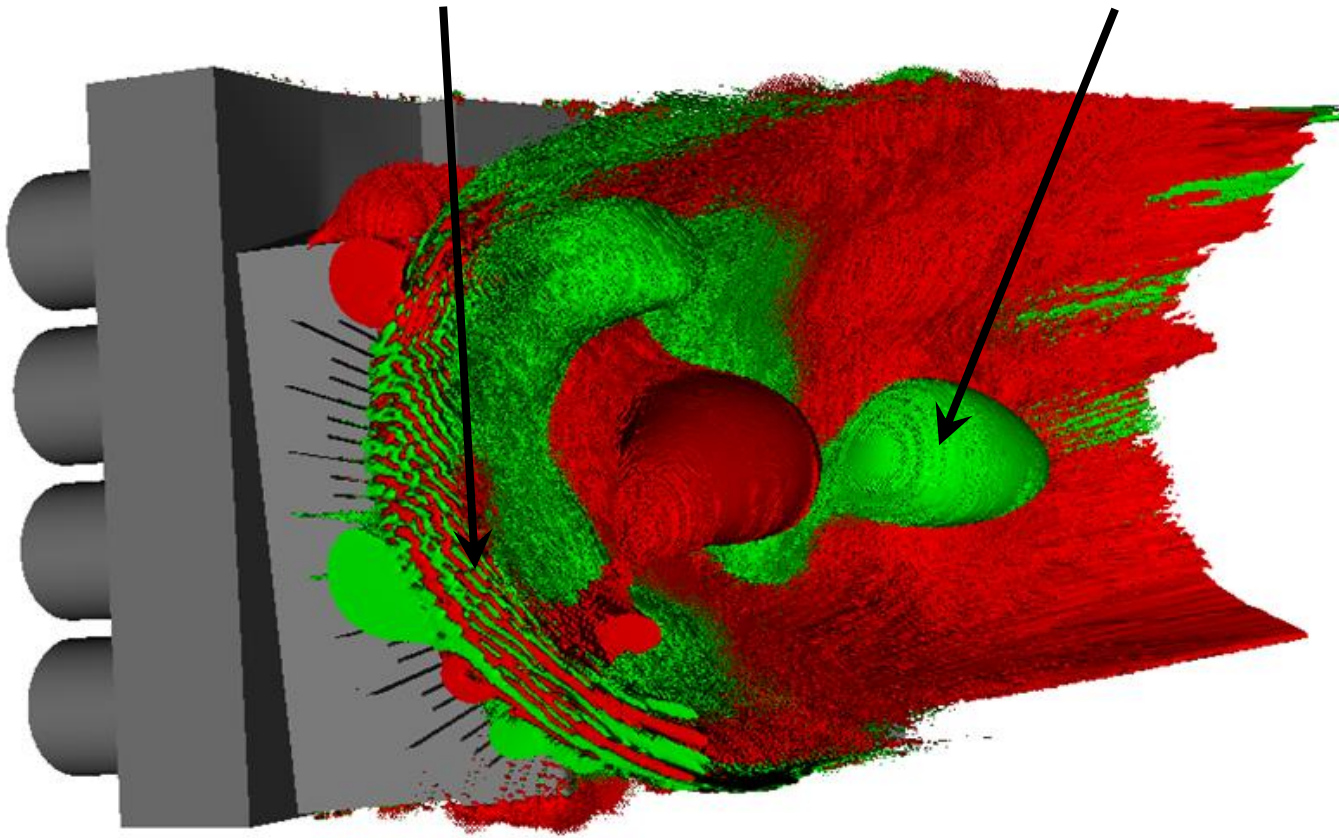
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Some RF Physics: Two Waves

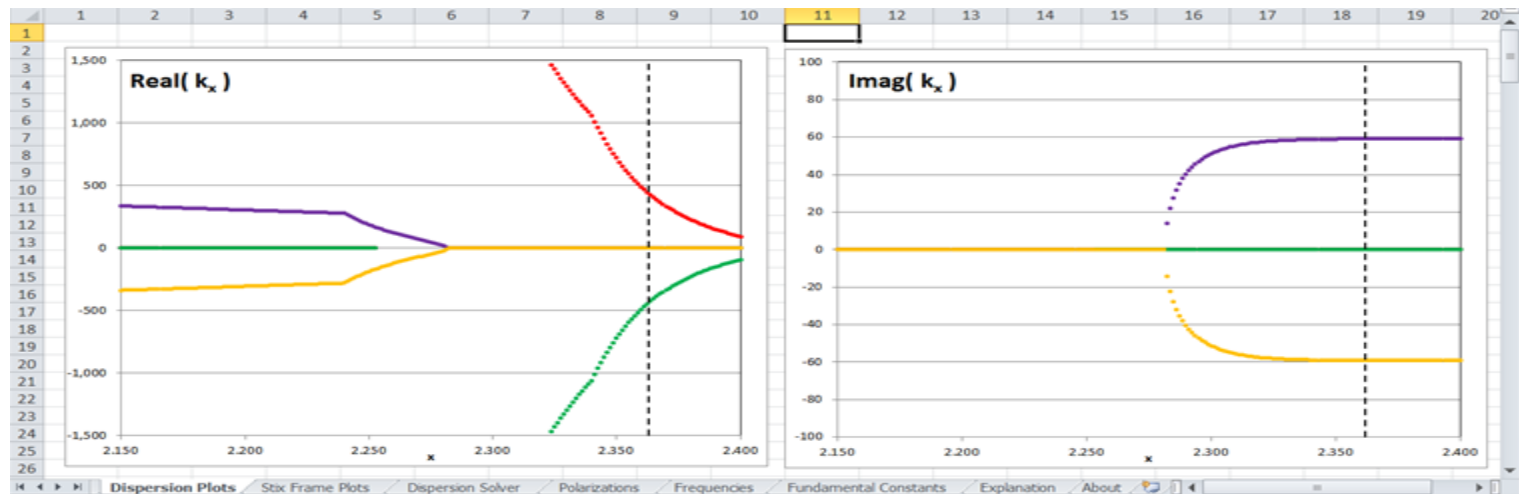
Slow Wave

Fast Wave



Two Waves, One Evanescent

- Nominally, the RF is excited in the “Fast” Wave, but has to tunnel through a 3-5 cm cut-off layer at the low edge density ($1 \times 10^{18} \text{m}^{-3}$), to get into the wave.
(On a good day.)
- If the density is too low ($3 \times 10^{17} \text{m}^{-3}$ for ICRH), then the slow wave is propagating, and propagates into a lower hybrid resonance a few cm's in front of the antenna.
(That's a bad day.)



Ponderomotive Force

- $| \text{Amplitude} |^2$ steady-state “wave pressure” from the RF’s $|E|^2$, $|B|^2$, and $|J_{\text{RF}}|^2$ energy, as it propagates through the steady-state plasma.
- Fast wave, $E \sim 3.0 \times 10^4 \text{ V/m} \rightarrow \text{Like } 0.05 \text{ eV}$
- Slow wave, $E \sim 1.5 \times 10^5 \text{ V/m} \rightarrow \text{Like } 1 \text{ eV}$
- If slow waves are present, **will they cause density rarefaction in front of antenna?**, thus perpetuating the low density that favors the slow wave. (**Chicken / Egg problem**).

VSim / BOUT++ Self Consistency

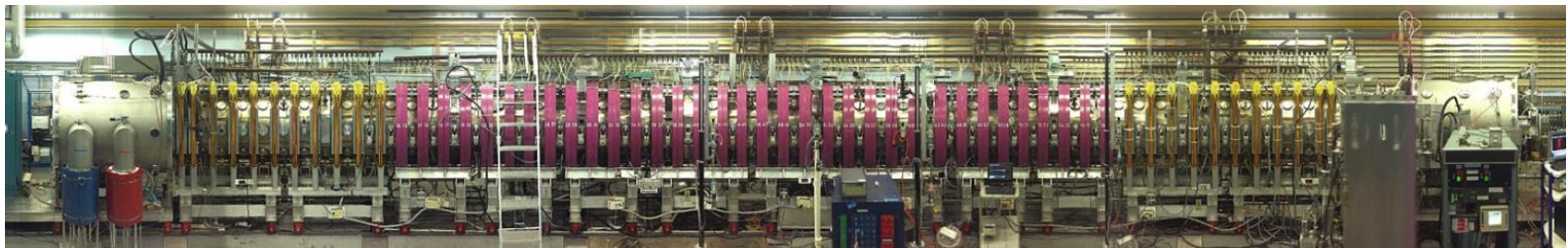
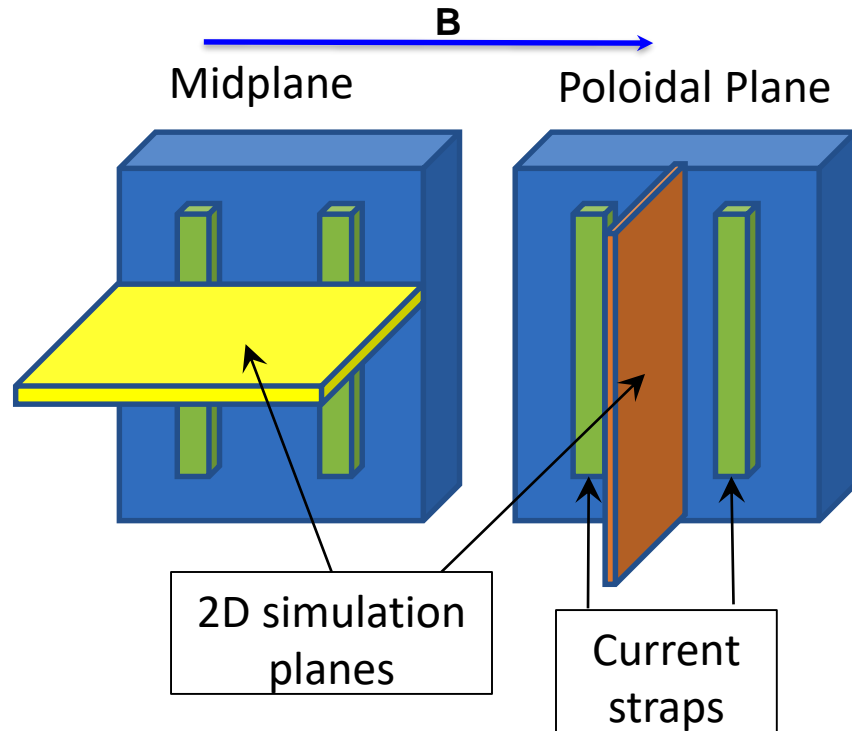
- Vorticity Equation uses $\mathbf{b} \times \mathbf{F}_{\text{ponderomotive}}$
 - Want to make sure we're using the same \mathbf{B}_0 field in VSim and BOUT++
- Since RF field amplitude depends critically on density in SOL / cutoff layer
 - Want to make sure we're using the same n_e profile in Vsim and BOUT++

Data Transfer and Workflow

- VSim \rightarrow BOUT++
 - Extra Ponderomotive Force
- BOUT++ \rightarrow VSim
 - Modified Density Profiles
- At first, data in files, manual runs.
 - VSim likes HDF5, BOUT++ likes NetCDF
 - python translation easy in VSim
- Later years ... maybe OMFIT or other run control.

Two Starting Geometries

- 2D runs can be either
 - midplane, or
 - poloidal plane.
- Midplane
 - Density rarefaction?
- Poloidal Plane
 - Convective cell?
- LAPD experiment.



Directed Case Studies

- Dominant Effect should be $-\rho_{s0} \nabla(\psi_p / Ze)$
e.g., *pushes away from large amplitudes.*
- Also want to set up a case of strong circularly polarized flow, to look at $\mathbf{B} \times (\nabla \times \mathbf{M})$ term.
- Also look at neutrals collision frequency terms

$$(q/m)_s \mathbf{F}_s = \frac{1}{2} (q/m)_s \text{Real} \{ \rho_{s1} \mathbf{E}_1^* + \mathbf{J}_{s1} \times \mathbf{B}_1^* \} - \frac{1}{2} \nabla \cdot [\rho_{s0}^{-1} \text{Real} \{ [\mathbf{J}_{s1} \mathbf{J}_{s1}^*] \}]$$

$$= -\frac{1}{4} \rho_{s0} \nabla(\rho_{s0}^{-2} |\mathbf{J}_{s1}|^2)$$

$$+ \frac{1}{2} \nabla \cdot [\mathbf{v}_s \rho_{s0}^{-1} \text{Imag} \{ [\mathbf{J}_{1s} \mathbf{J}_{s1}^*] \}] / \omega + \frac{1}{2} \mathbf{v}_s \rho_{s0}^{-1} \text{Imag} \{ [\nabla \mathbf{J}_{s1}] \cdot \mathbf{J}_{s1}^* \} / \omega$$

$$- \frac{1}{2} \nabla \cdot [\rho_{s0}^{-1} \text{Imag} \{ [\mathbf{J}_{1s} \mathbf{J}_{s1}^*] \} \times \boldsymbol{\Omega}_{s0}] / \omega + \frac{1}{4} \rho_{s0} \nabla(\rho_{s0}^{-2} \text{Imag} \{ \mathbf{J}_{s1} \times \mathbf{J}_{s1}^* \} \cdot \boldsymbol{\Omega}_{s0}) / \omega$$

Thank You

- Come back again at APS-DPP!
- Questions.